ABSTRACT

THESIS: Exchange Energy and Potential Using the Laplacian of the Density

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COLLEGE: Sciences and Humanities

DATE: May, 2012

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The challenge of density functional theory is the useful approximation of the exchange - correlation energy. This energy can be approximated with the local electron density and the gradient of the density. Many different generalized gradient approximations (GGA) have been made recently and there is controversy over the best overall functional. Recent Monte Carlo simulations give evidence that the Laplacian of the density might be a better starting place than the gradient to correct the local density approximation. We have tested several Laplacian based GGA models for exchange for small atoms. We use known constraints on the exchange energy used in current GGA's. In many models unphysical oscillations occur in the potential when using the Laplacian, and understanding and eliminating them is part of the focus of this research. We also find that mixing gradient and Laplacian seems to give a better result than only using one or the other.